Dimethyl ethylmalonate 26717-67-9 | DTXSID70181214

Model Performance

Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (7	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 4.14

Global applicability domain: Inside

Local applicability domain index: 9.83e-01

Confidence level: 7.89e-01

Nearest Neighbors from the Training Set

Image not found

Cumene

Measured: 3.98 Predicted: 3.95

Image not found

Benzonitrile

Measured: 4.46 Predicted: 3.95

Image not found

Nonene

Measured: 3.83 Predicted: 3.95

Image not found

Butyl ether

Measured: 3.89

Predicted: 3.93

Image not found

Hexyl acetate
Measured: 4.58
Predicted: 4.51